Programme

Faraday Discussion 162:
Fabrication, structure and reactivity of anchored nanoparticles
10-12 April, 2013
Berlin, Germany

Wednesday 10 April

11:00	**Registration, Tea and Coffee**
12:00	**Lunch**
	Session Chair: Gerhard Ertl
12.45	**Welcome and Introductions** Mike Bowker, *Cardiff University, UK*
13.00 **Paper 1**	**Introductory Lecture:** **Title TBC** Charles Campbell *University of Washington, USA*
Session 1	**Novel methods for nanoparticle fabrication** Session chair: Hans-Joachim Freund
14:00 **Paper 2**	**Exploring surface science and restructuring in reactive atmospheres of colloidally prepared bimetallic CuNi and CuCo nanoparticles on SiO_2 *in situ* using ambient pressure X-ray photoelectron spectroscopy** Simon Beaumont*, Selim Alayoglyu, Vladimir V Pushkarev, Shi Liu, Norbert Kruse and Gabor A Somorjai *University of California at Berkeley, USA*
Paper 3	**The structure of AuPd nanoalloys anchored on spherical polyelectrolyte brushes determined by X-ray absorption spectroscopy** Yan Lu*, Julian Kaiser, Wojciech Szczerba, Heinrich Riesemeier, Uwe Reinholz, Martin Radtke, Marting Albrecht and Matthias Ballauff *Helmholtz-Zentrum Berlin für Materialien und Energie, Germany*
Paper 4	**Semi-hydrogenation of alkynes at single crystal, nanoparticle and biogenic nanoparticle surfaces: the role of defects in Lindlar-type catalysts and the origin of their selectivity** Gary Attard*, J A Bennett, I Mikheenko, P Jenkins, S Guan, L E Macaski, J Wood and A J Wain *Cardiff University, UK*
15:30	Afternoon Tea
16:00 **Paper 5**	**Pt-group bimetallic nanocrystals with high-index facets as high performance electrocatalysts** Shi-Gang Sun*, Na Tian, Jing Xiao, Zhi-You Zhou, Hai-Xia Liu, Yu-Jia Deng, Long Huang and Bin-Bin Xu *Xiamen University, China*

Paper 6	**Shape-selected bimetallic nanoparticle electrocatalysts: evolution of their atomic-scale structure, chemical composition, and electrochemical reactivity under various chemical environments** Chunhua Cui, Lin Gan, Mahdi Ahmadi, Farzad Behafarid, Beatriz Roldan Cuenya, Max Neumann, Marc Heggen and Peter Strasser* *Technical University Berlin, Germany*
Paper 7	**Helium droplets: a new route to nanoparticles** Shengfu Yang*, Adrian Boatwright, Cheng Feng, Daniel Spence, Elspeth Latimer, Chris Binns and Andrew M Ellis *University of Leicester, UK*
17:30	Poster Session and Wine Reception
19:00	Dinner

Thursday 11 April

Session 2	**Surface science of anchored nanoparticles** Session Chair: Mike Bowker
09:00 **Paper 8**	**Charge competition with oxygen molecules determines the growth of gold particles on doped CaO films** Niklas Nilius*, Yi Cui, Kai Huang and Hans-Joachim Freund *FHI Berlin, Germany*
Paper 9	**Preparation and structure of a single Au atom on the TiO_2(110) surface: control of the Au-metal oxide surface interaction** Kiyotaka Asakura*, Satoru Takakusagi, Hiroko Ariga, Wang-Jae chun, Shushi Suzuki, Yuichico Koike, Hiromitsu Uehara, Kotaro Miyazaki and Yasuhiro Iwasawa *Hokkaido University, Japan*
10:00	Morning Coffee
10:30 **Paper 20**	***Operando* atomic structure and active sites of TiO_2(110)-supported gold nanoparticles during carbon monoxide oxidation** Marie-Claire Saint-Lager*, I Laoufi and A Bailly *Institut Néel – CNRS, France*
Paper 21	**CO and O overlayers on Pd nanocrystals supported on TiO_2(110)** Geoff Thornton*, Chi Ming Yim, Chi Lun Pang, David S Humphrey, Christopher A Muryn, Karina Sculte and Ruben Perez *University College London, UK*
Paper 17	**Fabrication of complex model oxide catalysts: Mo oxide on supported on Fe_3O_4 (111)** Philip R Davies*, Robert J Davies and Dyfan Edwards *Cardiff University, UK*
12:00	Close of Session & Lunch

Session 3	**Theoretical Approaches to Structure and Reactivity** Session Chair: Klaus Hermann
13:00 **Paper 10**	**Stability and migration barriers of small vanadium oxide clusters on the CeO2(111) surface studied by density functional theory** Joachim Paier*, Thomas Kropp, Christopher Penschke and Joachim Sauer *Humboldt Universität zu Berlin, Germany*
Paper 11	**Mechanistic insights into the partial oxidation of acetic acid by O_2 at the dual perimeter sites of a Au/TiO_2 catalyst** Matthew Neurock*, Isabel Xiaoye Green, Wenjie Tang and John T Yates Jnr *University of Virginia, USA*
Paper 12	**Catalyst nano-particle size dependence of Fischer-Tropsch reaction** Rutger van Santen* and Albert J Markvoort *Eindhoven University of Technology, The Netherlands*
14:30	Afternoon Tea
15:00 **Paper 13**	**A computational study of the influence of the ceria surface termination on the mechanism of CO oxidation of isolated Rh atoms** Emiel Hensen*, Weiyu Song and Tonek Jansen *Eindhoven University of Technology, The Netherlands*
Paper 14	**Morphology, dimension, and composition dependence of thermodynamically preferred atomic arrangements in Ag–Pt nanoalloys** Lei Deng*, Huiqui Deng, Shifang Xiao, Jianfeng Tang and Wangyu Hu *Hunan Agricultural University, China*
16:00	Close of sessions
19:00	Pre-Dinner Drinks
19:30	Conference Dinner

Friday 12 April

Session 4	**Reactivity of nanoparticles** Session chair: Gary Attard
09:30 **Paper 15**	**Alumina support and Pd_n cluster size effects on activity of Pd_n for catalytic oxidation of CO** Scott L Anderson*, Matthew D Kane and F Sloan Roberts *University of Utah, USA*
Paper 16	**Energetics of elementary reaction steps relevant for CO oxidation: CO and O_2 adsorption on model Pd nanoparticles and Pd (111)** Swetlana Schauermann*, Matthias Peter, Sergey Adamovsky and Jose Manuel Flores Camacho *FHI Berlin, Germany*
10:30	Morning Coffee
11:00 **Paper 18**	**Influence of hot carriers on catalytic reaction; Pt nanoparticles on GaN Substrates under light irradiation** Jeong Young Park*, Sun Mi Kim, Dahee Park, Youngji Yuk and Sang Hoon Kim *KAIST, Korea*
Paper 19	**Switching-off tolune formation in the solvent-free oxidation of benzyl alcohol using supported trimetallic Au-Pd-Pt nanoparticles** Qian He, Peter J Miedziak, Lokesh Kesavan, Nikos Dimitratos, Jennifer K. Edwards, Meenakshisundaram Sankar, Jose Antonio Lopez-Sanchez, Michael M Forde, David W Knight, Stuart H Taylor, Christopher J Kiely and Graham J Hutchings* *Cardiff University, UK*
	Close of session
12:00	**Concluding remarks lecture** Gabor Somorjai *University of California at Berkeley, USA*
12:45	**Acknowledgements**
13:00	Close of Meeting and Lunch